

Supplementary Material for
A perspective on molecular structure and
bonding-breaking in radiation damage in serial
femtosecond crystallography

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1 Input / output for CRETIN calculations associated with figure 1

1.1 Main input file

```
c -----  
c Aliases  
c -----  
alias N          3  
  
alias TE         0.01  
alias RHO        1.077  
  
alias E1         8000  
alias E2         E1 * 1.0104  
  
alias n0 1  
alias n1 3  
  
c CHEMICAL STOICHIOMETRY  
c PS1  
alias N_o 57.3e3 * RHO * AVGD / 13.13e5  
alias N_h 14.1e4 * RHO * AVGD / 13.13e5  
alias N_c 16.9e3 * RHO * AVGD / 13.13e5  
alias N_n 3310. * RHO * AVGD / 13.13e5  
alias N_s 89. * RHO * AVGD / 13.13e5  
alias N_mg 96. * RHO * AVGD / 13.13e5  
alias N_fe 12. * RHO * AVGD / 13.13e5  
alias N_ca 1. * RHO * AVGD / 13.13e5  
alias N_p 3. * RHO * AVGD / 13.13e5  
  
c LASER INTENSITY  
alias ILASER 2.000e+26  
c alias ILASER 1e7 * 5e14  
c [erg/cm2/s]  
  
c -----  
c Materials  
c -----  
  
atoms hydrogenic o  
atoms hydrogenic h  
atoms hydrogenic c  
atoms hydrogenic n
```

```
atoms hydrogenic s
atoms hydrogenic mg
atoms hydrogenic fe reconst
atoms hydrogenic ca
atoms hydrogenic p
```

```
c DEFINING THE MATERIAL REGIONS
```

```
c
region n0 n1 TE
element 1 N_o
element 2 N_h
element 3 N_c
element 4 N_n
element 5 N_s
element 6 N_mg
element 7 N_fe
element 8 N_ca
element 9 N_p
```

```
c -----
c   Radiation
c -----
```

```
angles 1
```

```
c SPECTRAL BINS, CAN BE REFINED CLOSE TO EDGES AND
c STRONG LINES
```

```
ebins 60 0.01 30.0
ebins 60 30.0 400.0
ebins 60 400.0 5.e4
```

```
c -----
c   Sources
c -----
```

```
alias MULT HPEV / ( E2 - E1)
```

```
c INCOMING LASER
```

```
source jbdry 1 E1 E2 value history 1 MULT
      xfilebc 1 1. 0. 1. 1          ! normal incidence, isotropy
```

```
c flat pulse
history 1 ILASER
tv 0. 1.
tv 1. 0.
```

```

c -----
c   Controls
c -----

tstart 0.
tquit 5.000e-14

c -----
c   Switches and Parameters
c -----

switch 11 1           ! make .plt file
switch 20 1           ! NLTE
switch 25 1           ! time-dependent

switch 28 0           ! LTE initialization
switch 31 1           ! temperature calculation
switch 44 250        ! maximum # of iterations

switch 72 1           ! timesteps between spectral calculations
switch 127 2
switch 126 10
switch 29 1

switch 125 1          ! average spectral emission over bins
switch 55 1            ! continuum lowering
switch 17 1           ! include line contributions in opacity
switch 36 1           ! turn on continuum transfer
switch 133 10002
switch 35 -1
switch 155 1
switch 146 1          ! turn on multiphoton ionization

param 40 1.e-15       ! time between edits
param 41 1.e-17       ! initial timestep
param 45 2.e-16       ! maximum timestep
param 61 1.e-3        ! iso-sequence population threshold
param 95 0.01         ! minimum Zbar for kinetics
param 102 0.01        ! minimum temperature

c -----
c   Edits
c -----

```

```
plot "depth vs zbar"  
  xvar r  
  yvar zbar 0:10
```

1.2 Raw output data

time = 0.0000E+00 : depth vs zbar
S r
zbar 1 zbar 2 zbar 3 zbar 4 zbar 5 zbar 6 zbar 7 zbar 8
0.000000E+00 1.000000E-02 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 1.000000E-02 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
0.000000E+00 1.000000E-02 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00 0.000000E+00
time = 0.0000E+00 : depth vs zbar
S r
zbar 9
0.000000E+00 0.000000E+00 1.000000E-02
0.000000E+00 0.000000E+00 1.000000E-02
0.000000E+00 0.000000E+00 1.000000E-02
time = 1.0000E-15 : depth vs zbar
S r
zbar 1 zbar 2 zbar 3 zbar 4 zbar 5 zbar 6 zbar 7 zbar 8
0.000000E+00 5.7720330E-01 8.9334322E-01 4.1164650E-01 8.3367375E-01 8.4763332E-01 6.7877839E-01 1.8067005E-01 2.8743392E+00 1.2426789E+00
0.000000E+00 5.7720330E-01 8.9334322E-01 4.1164650E-01 8.3367375E-01 8.4763332E-01 6.7877839E-01 1.8067005E-01 2.8743392E+00 1.2426789E+00
0.000000E+00 5.7720330E-01 8.9334322E-01 4.1164650E-01 8.3367375E-01 8.4763332E-01 6.7877839E-01 1.8067005E-01 2.8743392E+00 1.2426789E+00
time = 1.0000E-15 : depth vs zbar
S r
zbar 9
0.000000E+00 5.8164079E-01 5.7720330E-01
0.000000E+00 5.8164079E-01 5.7720330E-01
0.000000E+00 5.8164079E-01 5.7720330E-01
time = 2.0000E-15 : depth vs zbar
S r
zbar 1 zbar 2 zbar 3 zbar 4 zbar 5 zbar 6 zbar 7 zbar 8
0.000000E+00 7.9605739E-01 1.3729889E+00 4.9748832E-01 1.2219045E+00 1.3490563E+00 1.1457917E+00 2.4956722E-01 3.5597132E+00 1.5956296E+00
0.000000E+00 7.9605739E-01 1.3729889E+00 4.9748832E-01 1.2219045E+00 1.3490563E+00 1.1457917E+00 2.4956722E-01 3.5597132E+00 1.5956296E+00
0.000000E+00 7.9605739E-01 1.3729889E+00 4.9748832E-01 1.2219045E+00 1.3490563E+00 1.1457917E+00 2.4956722E-01 3.5597132E+00 1.5956296E+00
time = 2.0000E-15 : depth vs zbar
S r
zbar 9
0.000000E+00 8.6015840E-01 7.9605739E-01
0.000000E+00 8.6015840E-01 7.9605739E-01
0.000000E+00 8.6015840E-01 7.9605739E-01
time = 3.0000E-15 : depth vs zbar
S r
zbar 1 zbar 2 zbar 3 zbar 4 zbar 5 zbar 6 zbar 7 zbar 8
0.000000E+00 9.5375098E-01 1.7658442E+00 5.4757888E-01 1.4432894E+00 1.6918403E+00 1.4550926E+00 3.0659692E-01 4.0541753E+00 1.9242616E+00
0.000000E+00 9.5375098E-01 1.7658442E+00 5.4757888E-01 1.4432894E+00 1.6918403E+00 1.4550926E+00 3.0659692E-01 4.0541753E+00 1.9242616E+00
0.000000E+00 9.5375098E-01 1.7658442E+00 5.4757888E-01 1.4432894E+00 1.6918403E+00 1.4550926E+00 3.0659692E-01 4.0541753E+00 1.9242616E+00
time = 3.0000E-15 : depth vs zbar
S r
zbar 9
0.000000E+00 1.0815049E+00 9.5375098E-01
0.000000E+00 1.0815049E+00 9.5375098E-01
0.000000E+00 1.0815049E+00 9.5375098E-01
time = 4.0000E-15 : depth vs zbar
S r
zbar 1 zbar 2 zbar 3 zbar 4 zbar 5 zbar 6 zbar 7 zbar 8
0.000000E+00 1.0820605E+00 2.0880028E+00 5.8553077E-01 1.6398076E+00 1.9614814E+00 1.7379299E+00 3.7968483E-01 4.4693837E+00 2.2565982E+00
0.000000E+00 1.0820605E+00 2.0880028E+00 5.8553077E-01 1.6398076E+00 1.9614814E+00 1.7379299E+00 3.7968483E-01 4.4693837E+00 2.2565982E+00
0.000000E+00 1.0820605E+00 2.0880028E+00 5.8553077E-01 1.6398076E+00 1.9614814E+00 1.7379299E+00 3.7968483E-01 4.4693837E+00 2.2565982E+00
time = 4.0000E-15 : depth vs zbar
S r
zbar 9
0.000000E+00 1.2923184E+00 1.0820605E+00
0.000000E+00 1.2923184E+00 1.0820605E+00
0.000000E+00 1.2923184E+00 1.0820605E+00
time = 5.0000E-15 : depth vs zbar
S r
zbar 1 zbar 2 zbar 3 zbar 4 zbar 5 zbar 6 zbar 7 zbar 8
0.000000E+00 1.1875425E+00 1.3516837E+00 6.1585231E-01 1.8128451E+00 2.1794783E+00 2.0054768E+00 4.9180789E-01 4.8355265E+00 2.5823691E+00
0.000000E+00 1.1875425E+00 1.3516837E+00 6.1585231E-01 1.8128451E+00 2.1794783E+00 2.0054768E+00 4.9180789E-01 4.8355265E+00 2.5823691E+00
0.000000E+00 1.1875425E+00 1.3516837E+00 6.1585231E-01 1.8128451E+00 2.1794783E+00 2.0054768E+00 4.9180789E-01 4.8355265E+00 2.5823691E+00
time = 5.0000E-15 : depth vs zbar
S r
zbar 9
0.000000E+00 1.4954844E+00 1.1875425E+00
0.000000E+00 1.4954844E+00 1.1875425E+00
0.000000E+00 1.4954844E+00 1.1875425E+00
time = 6.0000E-15 : depth vs zbar
S r
zbar 1 zbar 2 zbar 3 zbar 4 zbar 5 zbar 6 zbar 7 zbar 8
0.000000E+00 1.2781590E+00 2.5767682E+00 6.4155141E-01 1.9687769E+00 2.3661723E+00 2.2649297E+00 6.6466232E-01 5.1779141E+00 2.9028095E+00
0.000000E+00 1.2781590E+00 2.5767682E+00 6.4155141E-01 1.9687769E+00 2.3661723E+00 2.2649297E+00 6.6466232E-01 5.1779141E+00 2.9028095E+00
0.000000E+00 1.2781590E+00 2.5767682E+00 6.4155141E-01 1.9687769E+00 2.3661723E+00 2.2649297E+00 6.6466232E-01 5.1779141E+00 2.9028095E+00
time = 6.0000E-15 : depth vs zbar
S r
zbar 9
0.000000E+00 1.6955189E+00 1.2781590E+00
0.000000E+00 1.6955189E+00 1.2781590E+00
0.000000E+00 1.6955189E+00 1.2781590E+00
time = 7.0000E-15 : depth vs zbar
S r
zbar 1 zbar 2 zbar 3 zbar 4 zbar 5 zbar 6 zbar 7 zbar 8
0.000000E+00 1.3578356E+00 2.7737926E+00 6.6391903E-01 2.1098616E+00 2.5314415E+00 2.5156200E+00 9.1776687E-01 5.5057644E+00 3.2130899E+00
0.000000E+00 1.3578356E+00 2.7737926E+00 6.6391903E-01 2.1098616E+00 2.5314415E+00 2.5156200E+00 9.1776687E-01 5.5057644E+00 3.2130899E+00
0.000000E+00 1.3578356E+00 2.7737926E+00 6.6391903E-01 2.1098616E+00 2.5314415E+00 2.5156200E+00 9.1776687E-01 5.5057644E+00 3.2130899E+00
time = 7.0000E-15 : depth vs zbar
S r
zbar 9
0.000000E+00 1.8930482E+00 1.3578356E+00
0.000000E+00 1.8930482E+00 1.3578356E+00
0.000000E+00 1.8930482E+00 1.3578356E+00
time = 8.0000E-15 : depth vs zbar
S r
zbar 1 zbar 2 zbar 3 zbar 4 zbar 5 zbar 6 zbar 7 zbar 8
0.000000E+00 1.4279905E+00 2.9468865E+00 6.8346544E-01 2.2359055E+00 2.6768834E+00 2.7415903E+00 1.2621471E+00 5.8159582E+00 3.5076985E+00
0.000000E+00 1.4279905E+00 2.9468865E+00 6.8346544E-01 2.2359055E+00 2.6768834E+00 2.7415903E+00 1.2621471E+00 5.8159582E+00 3.5076985E+00
0.000000E+00 1.4279905E+00 2.9468865E+00 6.8346544E-01 2.2359055E+00 2.6768834E+00 2.7415903E+00 1.2621471E+00 5.8159582E+00 3.5076985E+00
time = 8.0000E-15 : depth vs zbar
S r
zbar 9
0.000000E+00 2.0855275E+00 1.4279905E+00
0.000000E+00 2.0855275E+00 1.4279905E+00
0.000000E+00 2.0855275E+00 1.4279905E+00
time = 9.0000E-15 : depth vs zbar
S r
zbar 1 zbar 2 zbar 3 zbar 4 zbar 5 zbar 6 zbar 7 zbar 8
0.000000E+00 1.4905710E+00 3.1014150E+00 7.0071640E-01 2.3485781E+00 2.8078064E+00 2.9579362E+00 1.6938548E+00 6.1079219E+00 3.7845671E+00
0.000000E+00 1.4905710E+00 3.1014150E+00 7.0071640E-01 2.3485781E+00 2.8078064E+00 2.9579362E+00 1.6938548E+00 6.1079219E+00 3.7845671E+00
0.000000E+00 1.4905710E+00 3.1014150E+00 7.0071640E-01 2.3485781E+00 2.8078064E+00 2.9579362E+00 1.6938548E+00 6.1079219E+00 3.7845671E+00
time = 9.0000E-15 : depth vs zbar
S r
zbar 9
0.000000E+00 2.2723615E+00 1.4905710E+00
0.000000E+00 2.2723615E+00 1.4905710E+00
0.000000E+00 2.2723615E+00 1.4905710E+00
time = 1.0000E-14 : depth vs zbar
S r
zbar 1 zbar 2 zbar 3 zbar 4 zbar 5 zbar 6 zbar 7 zbar 8
0.000000E+00 1.5471257E+00 3.2415175E+00 7.1609101E-01 2.4496182E+00 2.9266716E+00 3.1651168E+00 2.1886042E+00 6.3818289E+00 4.0444580E+00
0.000000E+00 1.5471257E+00 3.2415175E+00 7.1609101E-01 2.4496182E+00 2.9266716E+00 3.1651168E+00 2.1886042E+00 6.3818289E+00 4.0444580E+00
0.000000E+00 1.5471257E+00 3.2415175E+00 7.1609101E-01 2.4496182E+00 2.9266716E+00 3.1651168E+00 2.1886042E+00 6.3818289E+00 4.0444580E+00
time = 1.0000E-14 : depth vs zbar
S r
zbar 9
0.000000E+00 2.4536526E+00 1.5471257E+00
0.000000E+00 2.4536526E+00 1.5471257E+00
0.000000E+00 2.4536526E+00 1.5471257E+00
time = 1.0000E-14 : depth vs zbar
S r
zbar 1 zbar 2 zbar 3 zbar 4 zbar 5 zbar 6 zbar 7 zbar 8
0.000000E+00 1.5987071E+00 3.7802611E+00 7.2989764E-01 2.5404773E+00 3.0368704E+00 3.3636269E+00 2.7027848E+00 6.6372509E+00 4.2883814E+00
0.000000E+00 1.5987071E+00 3.7802611E+00 7.2989764E-01 2.5404773E+00 3.0368704E+00 3.3636269E+00 2.7027848E+00 6.6372509E+00 4.2883814E+00
0.000000E+00 1.5987071E+00 3.7802611E+00 7.2989764E-01 2.5404773E+00 3.0368704E+00 3.3636269E+00 2.7027848E+00 6.6372509E+00 4.2883814E+00
time = 1.0000E-14 : depth vs zbar
S r
zbar 9
0.000000E+00 2.6297012E+00 1.5987071E+00
0.000000E+00 2.6297012E+00 1.5987071E+00
0.000000E+00 2.6297012E+00 1.5987071E+00

0.000000E+00 2.6297012E+00 1.5987071E+00
time = 1.2000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 1 2 3 4 5 6 7 8
0.000000E+00 1.6461269E+00 3.4890579E+00 7.4238441E-01 2.6224798E+00 3.1387320E+00 3.5537525E+00 3.1878035E+00 6.8750548E+00 4.5173528E+00
0.000000E+00 1.6461269E+00 3.4890579E+00 7.4238441E-01 2.6224798E+00 3.1387320E+00 3.5537525E+00 3.1878035E+00 6.8750548E+00 4.5173528E+00
0.000000E+00 1.6461269E+00 3.4890579E+00 7.4238441E-01 2.6224798E+00 3.1387320E+00 3.5537525E+00 3.1878035E+00 6.8750548E+00 4.5173528E+00
time = 1.2000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 9 10
0.000000E+00 2.7998461E+00 1.6461269E+00
0.000000E+00 2.7998461E+00 1.6461269E+00
0.000000E+00 2.7998461E+00 1.6461269E+00
time = 1.3000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 1 2 3 4 5 6 7 8
0.000000E+00 1.6900085E+00 3.6001737E+00 7.5374901E-01 2.6967761E+00 3.2331266E+00 3.7359034E+00 3.6086549E+00 7.0963232E+00 4.7328038E+00
0.000000E+00 1.6900085E+00 3.6001737E+00 7.5374901E-01 2.6967761E+00 3.2331266E+00 3.7359034E+00 3.6086549E+00 7.0963232E+00 4.7328038E+00
0.000000E+00 1.6900085E+00 3.6001737E+00 7.5374901E-01 2.6967761E+00 3.2331266E+00 3.7359034E+00 3.6086549E+00 7.0963232E+00 4.7328038E+00
time = 1.3000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 9 10
0.000000E+00 2.9650863E+00 1.6900085E+00
0.000000E+00 2.9650863E+00 1.6900085E+00
0.000000E+00 2.9650863E+00 1.6900085E+00
time = 1.4000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 1 2 3 4 5 6 7 8
0.000000E+00 1.7308431E+00 3.7045404E+00 7.6415100E-01 2.7643574E+00 3.3207964E+00 3.9105922E+00 3.9532379E+00 7.3020271E+00 4.9360267E+00
0.000000E+00 1.7308431E+00 3.7045404E+00 7.6415100E-01 2.7643574E+00 3.3207964E+00 3.9105922E+00 3.9532379E+00 7.3020271E+00 4.9360267E+00
0.000000E+00 1.7308431E+00 3.7045404E+00 7.6415100E-01 2.7643574E+00 3.3207964E+00 3.9105922E+00 3.9532379E+00 7.3020271E+00 4.9360267E+00
time = 1.4000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 9 10
0.000000E+00 3.1256751E+00 1.7308431E+00
0.000000E+00 3.1256751E+00 1.7308431E+00
0.000000E+00 3.1256751E+00 1.7308431E+00
time = 1.5000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 1 2 3 4 5 6 7 8
0.000000E+00 1.7690276E+00 3.8030454E+00 7.7372153E-01 2.8268012E+00 3.4023900E+00 4.0782672E+00 4.2290984E+00 7.4941998E+00 5.1345219E+00
0.000000E+00 1.7690276E+00 3.8030454E+00 7.7372153E-01 2.8268012E+00 3.4023900E+00 4.0782672E+00 4.2290984E+00 7.4941998E+00 5.1345219E+00
0.000000E+00 1.7690276E+00 3.8030454E+00 7.7372153E-01 2.8268012E+00 3.4023900E+00 4.0782672E+00 4.2290984E+00 7.4941998E+00 5.1345219E+00
time = 1.5000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 9 10
0.000000E+00 3.2843752E+00 1.7690276E+00
0.000000E+00 3.2843752E+00 1.7690276E+00
0.000000E+00 3.2843752E+00 1.7690276E+00
time = 1.6000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 1 2 3 4 5 6 7 8
0.000000E+00 1.8048812E+00 3.8963657E+00 7.8256797E-01 2.8826758E+00 3.4784710E+00 4.2401260E+00 4.4523823E+00 7.6749048E+00 5.3368492E+00
0.000000E+00 1.8048812E+00 3.8963657E+00 7.8256797E-01 2.8826758E+00 3.4784710E+00 4.2401260E+00 4.4523823E+00 7.6749048E+00 5.3368492E+00
0.000000E+00 1.8048812E+00 3.8963657E+00 7.8256797E-01 2.8826758E+00 3.4784710E+00 4.2401260E+00 4.4523823E+00 7.6749048E+00 5.3368492E+00
time = 1.6000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 9 10
0.000000E+00 3.4418556E+00 1.8048812E+00
0.000000E+00 3.4418556E+00 1.8048812E+00
0.000000E+00 3.4418556E+00 1.8048812E+00
time = 1.7000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 1 2 3 4 5 6 7 8
0.000000E+00 1.8386645E+00 3.9858312E+00 7.9078080E-01 2.9347736E+00 3.5495449E+00 4.3965032E+00 4.6389014E+00 7.8463239E+00 5.5390430E+00
0.000000E+00 1.8386645E+00 3.9858312E+00 7.9078080E-01 2.9347736E+00 3.5495449E+00 4.3965032E+00 4.6389014E+00 7.8463239E+00 5.5390430E+00
0.000000E+00 1.8386645E+00 3.9858312E+00 7.9078080E-01 2.9347736E+00 3.5495449E+00 4.3965032E+00 4.6389014E+00 7.8463239E+00 5.5390430E+00
time = 1.7000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 9 10
0.000000E+00 3.5978140E+00 1.8386645E+00
0.000000E+00 3.5978140E+00 1.8386645E+00
0.000000E+00 3.5978140E+00 1.8386645E+00
time = 1.8000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 1 2 3 4 5 6 7 8
0.000000E+00 1.8705929E+00 4.0694657E+00 7.9843621E-01 2.9829195E+00 3.6160639E+00 4.5482029E+00 4.8010975E+00 8.0108318E+00 5.7422659E+00
0.000000E+00 1.8705929E+00 4.0694657E+00 7.9843621E-01 2.9829195E+00 3.6160639E+00 4.5482029E+00 4.8010975E+00 8.0108318E+00 5.7422659E+00
0.000000E+00 1.8705929E+00 4.0694657E+00 7.9843621E-01 2.9829195E+00 3.6160639E+00 4.5482029E+00 4.8010975E+00 8.0108318E+00 5.7422659E+00
time = 1.8000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 9 10
0.000000E+00 3.7547250E+00 1.8705929E+00
0.000000E+00 3.7547250E+00 1.8705929E+00
0.000000E+00 3.7547250E+00 1.8705929E+00
time = 1.9000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 1 2 3 4 5 6 7 8
0.000000E+00 1.9008437E+00 4.1500112E+00 8.0559872E-01 3.0275833E+00 3.6784212E+00 4.6960022E+00 4.9475133E+00 8.1701742E+00 5.9483690E+00
0.000000E+00 1.9008437E+00 4.1500112E+00 8.0559872E-01 3.0275833E+00 3.6784212E+00 4.6960022E+00 4.9475133E+00 8.1701742E+00 5.9483690E+00
0.000000E+00 1.9008437E+00 4.1500112E+00 8.0559872E-01 3.0275833E+00 3.6784212E+00 4.6960022E+00 4.9475133E+00 8.1701742E+00 5.9483690E+00
time = 1.9000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 9 10
0.000000E+00 3.9118062E+00 1.9008437E+00
0.000000E+00 3.9118062E+00 1.9008437E+00
0.000000E+00 3.9118062E+00 1.9008437E+00
time = 2.0000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 1 2 3 4 5 6 7 8
0.000000E+00 1.9295657E+00 4.2269489E+00 8.1232303E-01 3.0691712E+00 3.7369846E+00 4.8406765E+00 5.0835100E+00 8.3264377E+00 6.1575057E+00
0.000000E+00 1.9295657E+00 4.2269489E+00 8.1232303E-01 3.0691712E+00 3.7369846E+00 4.8406765E+00 5.0835100E+00 8.3264377E+00 6.1575057E+00
0.000000E+00 1.9295657E+00 4.2269489E+00 8.1232303E-01 3.0691712E+00 3.7369846E+00 4.8406765E+00 5.0835100E+00 8.3264377E+00 6.1575057E+00
time = 2.0000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 9 10
0.000000E+00 4.0692618E+00 1.9295657E+00
0.000000E+00 4.0692618E+00 1.9295657E+00
0.000000E+00 4.0692618E+00 1.9295657E+00
time = 2.1000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 1 2 3 4 5 6 7 8
0.000000E+00 1.9568901E+00 4.3005208E+00 8.1865766E-01 3.1080457E+00 3.7920998E+00 4.9023479E+00 5.2124762E+00 8.4847323E+00 6.3713794E+00
0.000000E+00 1.9568901E+00 4.3005208E+00 8.1865766E-01 3.1080457E+00 3.7920998E+00 4.9023479E+00 5.2124762E+00 8.4847323E+00 6.3713794E+00
0.000000E+00 1.9568901E+00 4.3005208E+00 8.1865766E-01 3.1080457E+00 3.7920998E+00 4.9023479E+00 5.2124762E+00 8.4847323E+00 6.3713794E+00
time = 2.1000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 9 10
0.000000E+00 4.2272628E+00 1.9568901E+00
0.000000E+00 4.2272628E+00 1.9568901E+00
0.000000E+00 4.2272628E+00 1.9568901E+00
time = 2.2000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 1 2 3 4 5 6 7 8
0.000000E+00 1.9829306E+00 4.3709545E+00 8.2464171E-01 3.1445101E+00 3.8440570E+00 5.1234100E+00 5.3442750E+00 8.6445451E+00 6.5904671E+00
0.000000E+00 1.9829306E+00 4.3709545E+00 8.2464171E-01 3.1445101E+00 3.8440570E+00 5.1234100E+00 5.3442750E+00 8.6445451E+00 6.5904671E+00
0.000000E+00 1.9829306E+00 4.3709545E+00 8.2464171E-01 3.1445101E+00 3.8440570E+00 5.1234100E+00 5.3442750E+00 8.6445451E+00 6.5904671E+00
time = 2.2000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 9 10
0.000000E+00 4.3859103E+00 1.9829306E+00
0.000000E+00 4.3859103E+00 1.9829306E+00
0.000000E+00 4.3859103E+00 1.9829306E+00
time = 2.3000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 1 2 3 4 5 6 7 8
0.000000E+00 2.0077651E+00 4.4383871E+00 8.3030837E-01 3.1788245E+00 3.8931018E+00 5.2634231E+00 5.4621873E+00 8.8072135E+00 6.8148374E+00
0.000000E+00 2.0077651E+00 4.4383871E+00 8.3030837E-01 3.1788245E+00 3.8931018E+00 5.2634231E+00 5.4621873E+00 8.8072135E+00 6.8148374E+00
0.000000E+00 2.0077651E+00 4.4383871E+00 8.3030837E-01 3.1788245E+00 3.8931018E+00 5.2634231E+00 5.4621873E+00 8.8072135E+00 6.8148374E+00
time = 2.3000E-14 : depth vs zbar
\$ r zbar zbar zbar zbar zbar zbar zbar zbar
\$ 9 10

```

S
9 10
0.000000E+00 4.5452062E+00 2.0077651E+00
0.000000E+00 4.5452062E+00 2.0077651E+00
0.000000E+00 4.5452062E+00 2.0077651E+00
# time = 2.4000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 1 2 3 4 5 6 7 8
0.000000E+00 2.0314763E+00 4.5029698E+00 8.3568608E-01 3.2112191E+00 3.9394601E+00 5.4030142E+00 5.5773976E+00 8.9736605E+00 7.0450561E+00
0.000000E+00 2.0314763E+00 4.5029698E+00 8.3568608E-01 3.2112191E+00 3.9394601E+00 5.4030142E+00 5.5773976E+00 8.9736605E+00 7.0450561E+00
0.000000E+00 2.0314763E+00 4.5029698E+00 8.3568608E-01 3.2112191E+00 3.9394601E+00 5.4030142E+00 5.5773976E+00 8.9736605E+00 7.0450561E+00
# time = 2.4000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 9 10
0.000000E+00 4.7055585E+00 2.0314763E+00
0.000000E+00 4.7055585E+00 2.0314763E+00
0.000000E+00 4.7055585E+00 2.0314763E+00
# time = 2.5000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 1 2 3 4 5 6 7 8
0.000000E+00 2.0541345E+00 4.5648322E+00 8.4079987E-01 3.2418997E+00 3.9833385E+00 5.5426845E+00 5.6903286E+00 9.1451491E+00 7.2802739E+00
0.000000E+00 2.0541345E+00 4.5648322E+00 8.4079987E-01 3.2418997E+00 3.9833385E+00 5.5426845E+00 5.6903286E+00 9.1451491E+00 7.2802739E+00
0.000000E+00 2.0541345E+00 4.5648322E+00 8.4079987E-01 3.2418997E+00 3.9833385E+00 5.5426845E+00 5.6903286E+00 9.1451491E+00 7.2802739E+00
# time = 2.5000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 9 10
0.000000E+00 4.8667470E+00 2.0541345E+00
0.000000E+00 4.8667470E+00 2.0541345E+00
0.000000E+00 4.8667470E+00 2.0541345E+00
# time = 2.6000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 1 2 3 4 5 6 7 8
0.000000E+00 2.0758393E+00 4.6242604E+00 8.4566611E-01 3.2718256E+00 4.0248922E+00 5.6827899E+00 5.8008677E+00 9.3216532E+00 7.5195475E+00
0.000000E+00 2.0758393E+00 4.6242604E+00 8.4566611E-01 3.2718256E+00 4.0248922E+00 5.6827899E+00 5.8008677E+00 9.3216532E+00 7.5195475E+00
0.000000E+00 2.0758393E+00 4.6242604E+00 8.4566611E-01 3.2718256E+00 4.0248922E+00 5.6827899E+00 5.8008677E+00 9.3216532E+00 7.5195475E+00
# time = 2.6000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 9 10
0.000000E+00 5.0286955E+00 2.0758393E+00
0.000000E+00 5.0286955E+00 2.0758393E+00
0.000000E+00 5.0286955E+00 2.0758393E+00
# time = 2.7000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 1 2 3 4 5 6 7 8
0.000000E+00 2.0956540E+00 4.6809989E+00 8.5031516E-01 3.2988114E+00 4.0643552E+00 5.8236793E+00 5.9809560E+00 9.5041891E+00 7.7627022E+00
0.000000E+00 2.0956540E+00 4.6809989E+00 8.5031516E-01 3.2988114E+00 4.0643552E+00 5.8236793E+00 5.9809560E+00 9.5041891E+00 7.7627022E+00
0.000000E+00 2.0956540E+00 4.6809989E+00 8.5031516E-01 3.2988114E+00 4.0643552E+00 5.8236793E+00 5.9809560E+00 9.5041891E+00 7.7627022E+00
# time = 2.7000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 9 10
0.000000E+00 5.1914298E+00 2.0956540E+00
0.000000E+00 5.1914298E+00 2.0956540E+00
0.000000E+00 5.1914298E+00 2.0956540E+00
# time = 2.8000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 1 2 3 4 5 6 7 8
0.000000E+00 2.1164065E+00 4.7353626E+00 8.5475624E-01 3.3253717E+00 4.1018366E+00 5.9644802E+00 6.0145551E+00 9.6931595E+00 8.0092064E+00
0.000000E+00 2.1164065E+00 4.7353626E+00 8.5475624E-01 3.3253717E+00 4.1018366E+00 5.9644802E+00 6.0145551E+00 9.6931595E+00 8.0092064E+00
0.000000E+00 2.1164065E+00 4.7353626E+00 8.5475624E-01 3.3253717E+00 4.1018366E+00 5.9644802E+00 6.0145551E+00 9.6931595E+00 8.0092064E+00
# time = 2.8000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 9 10
0.000000E+00 5.3548407E+00 2.1164065E+00
0.000000E+00 5.3548407E+00 2.1164065E+00
0.000000E+00 5.3548407E+00 2.1164065E+00
# time = 2.9000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 1 2 3 4 5 6 7 8
0.000000E+00 2.1354133E+00 4.7874389E+00 8.5900373E-01 3.3508396E+00 4.1374745E+00 6.1076589E+00 6.1176781E+00 9.8891161E+00 8.2575870E+00
0.000000E+00 2.1354133E+00 4.7874389E+00 8.5900373E-01 3.3508396E+00 4.1374745E+00 6.1076589E+00 6.1176781E+00 9.8891161E+00 8.2575870E+00
0.000000E+00 2.1354133E+00 4.7874389E+00 8.5900373E-01 3.3508396E+00 4.1374745E+00 6.1076589E+00 6.1176781E+00 9.8891161E+00 8.2575870E+00
# time = 2.9000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 9 10
0.000000E+00 5.5187948E+00 2.1354133E+00
0.000000E+00 5.5187948E+00 2.1354133E+00
0.000000E+00 5.5187948E+00 2.1354133E+00
# time = 3.0000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 1 2 3 4 5 6 7 8
0.000000E+00 2.1536263E+00 4.8373186E+00 8.6307020E-01 3.3753360E+00 4.1713935E+00 6.2517490E+00 6.2182926E+00 1.0092250E+01 8.5050132E+00
0.000000E+00 2.1536263E+00 4.8373186E+00 8.6307020E-01 3.3753360E+00 4.1713935E+00 6.2517490E+00 6.2182926E+00 1.0092250E+01 8.5050132E+00
0.000000E+00 2.1536263E+00 4.8373186E+00 8.6307020E-01 3.3753360E+00 4.1713935E+00 6.2517490E+00 6.2182926E+00 1.0092250E+01 8.5050132E+00
# time = 3.0000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 9 10
0.000000E+00 5.6833052E+00 2.1536263E+00
0.000000E+00 5.6833052E+00 2.1536263E+00
0.000000E+00 5.6833052E+00 2.1536263E+00
# time = 3.1000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 1 2 3 4 5 6 7 8
0.000000E+00 2.1710857E+00 4.8850875E+00 8.6696676E-01 3.3989714E+00 4.2037078E+00 6.3966261E+00 6.3163829E+00 1.0302869E+01 8.7545527E+00
0.000000E+00 2.1710857E+00 4.8850875E+00 8.6696676E-01 3.3989714E+00 4.2037078E+00 6.3966261E+00 6.3163829E+00 1.0302869E+01 8.7545527E+00
0.000000E+00 2.1710857E+00 4.8850875E+00 8.6696676E-01 3.3989714E+00 4.2037078E+00 6.3966261E+00 6.3163829E+00 1.0302869E+01 8.7545527E+00
# time = 3.1000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 9 10
0.000000E+00 5.8480221E+00 2.1710857E+00
0.000000E+00 5.8480221E+00 2.1710857E+00
0.000000E+00 5.8480221E+00 2.1710857E+00
# time = 3.2000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 1 2 3 4 5 6 7 8
0.000000E+00 2.1878289E+00 4.9308294E+00 8.7070317E-01 3.4218472E+00 4.2345214E+00 6.5420605E+00 6.4119806E+00 1.0521481E+01 9.0028090E+00
0.000000E+00 2.1878289E+00 4.9308294E+00 8.7070317E-01 3.4218472E+00 4.2345214E+00 6.5420605E+00 6.4119806E+00 1.0521481E+01 9.0028090E+00
0.000000E+00 2.1878289E+00 4.9308294E+00 8.7070317E-01 3.4218472E+00 4.2345214E+00 6.5420605E+00 6.4119806E+00 1.0521481E+01 9.0028090E+00
# time = 3.2000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 9 10
0.000000E+00 6.0124859E+00 2.1878289E+00
0.000000E+00 6.0124859E+00 2.1878289E+00
0.000000E+00 6.0124859E+00 2.1878289E+00
# time = 3.3000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 1 2 3 4 5 6 7 8
0.000000E+00 2.2038913E+00 4.9746247E+00 8.7428828E-01 3.4440581E+00 4.2639309E+00 6.6877398E+00 6.5049104E+00 1.0747535E+01 9.2496920E+00
0.000000E+00 2.2038913E+00 4.9746247E+00 8.7428828E-01 3.4440581E+00 4.2639309E+00 6.6877398E+00 6.5049104E+00 1.0747535E+01 9.2496920E+00
0.000000E+00 2.2038913E+00 4.9746247E+00 8.7428828E-01 3.4440581E+00 4.2639309E+00 6.6877398E+00 6.5049104E+00 1.0747535E+01 9.2496920E+00
# time = 3.3000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 9 10
0.000000E+00 6.1763119E+00 2.2038913E+00
0.000000E+00 6.1763119E+00 2.2038913E+00
0.000000E+00 6.1763119E+00 2.2038913E+00
# time = 3.4000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 1 2 3 4 5 6 7 8
0.000000E+00 2.2193068E+00 5.0165516E+00 8.772998E-01 3.4656918E+00 4.2920257E+00 6.8343195E+00 6.5952398E+00 1.0981386E+01 9.4926723E+00
0.000000E+00 2.2193068E+00 5.0165516E+00 8.772998E-01 3.4656918E+00 4.2920257E+00 6.8343195E+00 6.5952398E+00 1.0981386E+01 9.4926723E+00
0.000000E+00 2.2193068E+00 5.0165516E+00 8.772998E-01 3.4656918E+00 4.2920257E+00 6.8343195E+00 6.5952398E+00 1.0981386E+01 9.4926723E+00
# time = 3.4000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 9 10
0.000000E+00 6.3390373E+00 2.2193068E+00
0.000000E+00 6.3390373E+00 2.2193068E+00
0.000000E+00 6.3390373E+00 2.2193068E+00
# time = 3.5000E-14 : depth vs zbar
S r zbar zbar zbar zbar zbar zbar zbar zbar
S 1 2 3 4 5 6 7 8
0.000000E+00 2.2341070E+00 5.0566871E+00 8.8103551E-01 3.4868305E+00 4.3188893E+00 6.9794174E+00 6.6829599E+00 1.1222983E+01 9.7320952E+00
0.000000E+00 2.2341070E+00 5.0566871E+00 8.8103551E-01 3.4868305E+00 4.3188893E+00 6.9794174E+00 6.6829599E+00 1.1222983E+01 9.7320952E+00
0.000000E+00 2.2341070E+00 5.0566871E+00 8.8103551E-01 3.4868305E+00 4.3188893E+00 6.9794174E+00 6.6829599E+00 1.1222983E+01 9.7320952E+00

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```
# time = 3.5000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 9 10
0.000000E+00 6.5001500E+00 2.2341070E+00
0.000000E+00 6.5001500E+00 2.2341070E+00
0.000000E+00 6.5001500E+00 2.2341070E+00
# time = 3.6000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 1 2 3 4 5 6 7 8
0.000000E+00 2.2483233E+00 5.0951081E+00 8.8421123E-01 3.5075502E+00 4.3445980E+00 7.1236356E+00 6.7680710E+00 1.1472198E+01 9.9673557E+00
0.000000E+00 2.2483233E+00 5.0951081E+00 8.8421123E-01 3.5075502E+00 4.3445980E+00 7.1236356E+00 6.7680710E+00 1.1472198E+01 9.9673557E+00
0.000000E+00 2.2483233E+00 5.0951081E+00 8.8421123E-01 3.5075502E+00 4.3445980E+00 7.1236356E+00 6.7680710E+00 1.1472198E+01 9.9673557E+00
# time = 3.6000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 9 10
0.000000E+00 6.6593255E+00 2.2483233E+00
0.000000E+00 6.6593255E+00 2.2483233E+00
0.000000E+00 6.6593255E+00 2.2483233E+00
# time = 3.7000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 1 2 3 4 5 6 7 8
0.000000E+00 2.2619852E+00 5.1318871E+00 8.8726310E-01 3.5279229E+00 4.3692247E+00 7.2665558E+00 6.8505925E+00 1.1728896E+01 1.0197986E+01
0.000000E+00 2.2619852E+00 5.1318871E+00 8.8726310E-01 3.5279229E+00 4.3692247E+00 7.2665558E+00 6.8505925E+00 1.1728896E+01 1.0197986E+01
0.000000E+00 2.2619852E+00 5.1318871E+00 8.8726310E-01 3.5279229E+00 4.3692247E+00 7.2665558E+00 6.8505925E+00 1.1728896E+01 1.0197986E+01
# time = 3.7000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 9 10
0.000000E+00 6.8159227E+00 2.2619852E+00
0.000000E+00 6.8159227E+00 2.2619852E+00
0.000000E+00 6.8159227E+00 2.2619852E+00
# time = 3.8000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 1 2 3 4 5 6 7 8
0.000000E+00 2.2751206E+00 5.1670947E+00 8.9019665E-01 3.5480163E+00 4.3928376E+00 7.4077903E+00 6.9305601E+00 1.1992730E+01 1.0423655E+01
0.000000E+00 2.2751206E+00 5.1670947E+00 8.9019665E-01 3.5480163E+00 4.3928376E+00 7.4077903E+00 6.9305601E+00 1.1992730E+01 1.0423655E+01
0.000000E+00 2.2751206E+00 5.1670947E+00 8.9019665E-01 3.5480163E+00 4.3928376E+00 7.4077903E+00 6.9305601E+00 1.1992730E+01 1.0423655E+01
# time = 3.8000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 9 10
0.000000E+00 6.9693992E+00 2.2751206E+00
0.000000E+00 6.9693992E+00 2.2751206E+00
0.000000E+00 6.9693992E+00 2.2751206E+00
# time = 3.9000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 1 2 3 4 5 6 7 8
0.000000E+00 2.2877590E+00 5.2007984E+00 8.9301674E-01 3.5678928E+00 4.4156930E+00 7.5470023E+00 7.0880257E+00 1.2263364E+01 1.0644160E+01
0.000000E+00 2.2877590E+00 5.2007984E+00 8.9301674E-01 3.5678928E+00 4.4156930E+00 7.5470023E+00 7.0880257E+00 1.2263364E+01 1.0644160E+01
0.000000E+00 2.2877590E+00 5.2007984E+00 8.9301674E-01 3.5678928E+00 4.4156930E+00 7.5470023E+00 7.0880257E+00 1.2263364E+01 1.0644160E+01
# time = 3.9000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 9 10
0.000000E+00 7.1193018E+00 2.2877590E+00
0.000000E+00 7.1193018E+00 2.2877590E+00
0.000000E+00 7.1193018E+00 2.2877590E+00
# time = 4.0000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 1 2 3 4 5 6 7 8
0.000000E+00 2.2999221E+00 5.2330691E+00 8.9572859E-01 3.5876140E+00 4.4374432E+00 7.6847895E+00 7.0830592E+00 1.2540644E+01 1.0859401E+01
0.000000E+00 2.2999221E+00 5.2330691E+00 8.9572859E-01 3.5876140E+00 4.4374432E+00 7.6847895E+00 7.0830592E+00 1.2540644E+01 1.0859401E+01
0.000000E+00 2.2999221E+00 5.2330691E+00 8.9572859E-01 3.5876140E+00 4.4374432E+00 7.6847895E+00 7.0830592E+00 1.2540644E+01 1.0859401E+01
# time = 4.0000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 9 10
0.000000E+00 7.2662366E+00 2.2999221E+00
0.000000E+00 7.2662366E+00 2.2999221E+00
0.000000E+00 7.2662366E+00 2.2999221E+00
# time = 4.1000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 1 2 3 4 5 6 7 8
0.000000E+00 2.3116370E+00 5.2639707E+00 8.9833640E-01 3.6072346E+00 4.4583659E+00 7.8190521E+00 7.1557479E+00 1.2823561E+01 1.1069975E+01
0.000000E+00 2.3116370E+00 5.2639707E+00 8.9833640E-01 3.6072346E+00 4.4583659E+00 7.8190521E+00 7.1557479E+00 1.2823561E+01 1.1069975E+01
0.000000E+00 2.3116370E+00 5.2639707E+00 8.9833640E-01 3.6072346E+00 4.4583659E+00 7.8190521E+00 7.1557479E+00 1.2823561E+01 1.1069975E+01
# time = 4.1000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 9 10
0.000000E+00 7.4077734E+00 2.3116370E+00
0.000000E+00 7.4077734E+00 2.3116370E+00
0.000000E+00 7.4077734E+00 2.3116370E+00
# time = 4.2000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 1 2 3 4 5 6 7 8
0.000000E+00 2.3229281E+00 5.2935669E+00 9.0084433E-01 3.6268065E+00 4.4785150E+00 7.9506886E+00 7.2261926E+00 1.3111749E+01 1.1274580E+01
0.000000E+00 2.3229281E+00 5.2935669E+00 9.0084433E-01 3.6268065E+00 4.4785150E+00 7.9506886E+00 7.2261926E+00 1.3111749E+01 1.1274580E+01
0.000000E+00 2.3229281E+00 5.2935669E+00 9.0084433E-01 3.6268065E+00 4.4785150E+00 7.9506886E+00 7.2261926E+00 1.3111749E+01 1.1274580E+01
# time = 4.2000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 9 10
0.000000E+00 7.5448793E+00 2.3229281E+00
0.000000E+00 7.5448793E+00 2.3229281E+00
0.000000E+00 7.5448793E+00 2.3229281E+00
# time = 4.3000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 1 2 3 4 5 6 7 8
0.000000E+00 2.3338187E+00 5.3219195E+00 9.0325632E-01 3.6463780E+00 4.4979423E+00 8.0796216E+00 7.2945061E+00 1.3404635E+01 1.1474181E+01
0.000000E+00 2.3338187E+00 5.3219195E+00 9.0325632E-01 3.6463780E+00 4.4979423E+00 8.0796216E+00 7.2945061E+00 1.3404635E+01 1.1474181E+01
0.000000E+00 2.3338187E+00 5.3219195E+00 9.0325632E-01 3.6463780E+00 4.4979423E+00 8.0796216E+00 7.2945061E+00 1.3404635E+01 1.1474181E+01
# time = 4.3000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 9 10
0.000000E+00 7.6774454E+00 2.3338187E+00
0.000000E+00 7.6774454E+00 2.3338187E+00
0.000000E+00 7.6774454E+00 2.3338187E+00
# time = 4.4000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 1 2 3 4 5 6 7 8
0.000000E+00 2.3443313E+00 5.3490886E+00 9.0557615E-01 3.6659941E+00 4.5166972E+00 8.2058410E+00 7.3608097E+00 1.3701693E+01 1.1668966E+01
0.000000E+00 2.3443313E+00 5.3490886E+00 9.0557615E-01 3.6659941E+00 4.5166972E+00 8.2058410E+00 7.3608097E+00 1.3701693E+01 1.1668966E+01
0.000000E+00 2.3443313E+00 5.3490886E+00 9.0557615E-01 3.6659941E+00 4.5166972E+00 8.2058410E+00 7.3608097E+00 1.3701693E+01 1.1668966E+01
# time = 4.4000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 9 10
0.000000E+00 7.8054758E+00 2.3443313E+00
0.000000E+00 7.8054758E+00 2.3443313E+00
0.000000E+00 7.8054758E+00 2.3443313E+00
# time = 4.5000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 1 2 3 4 5 6 7 8
0.000000E+00 2.3544877E+00 5.3751321E+00 9.0780735E-01 3.6856958E+00 4.5348266E+00 8.3303180E+00 7.4253452E+00 1.4002219E+01 1.1858903E+01
0.000000E+00 2.3544877E+00 5.3751321E+00 9.0780735E-01 3.6856958E+00 4.5348266E+00 8.3303180E+00 7.4253452E+00 1.4002219E+01 1.1858903E+01
0.000000E+00 2.3544877E+00 5.3751321E+00 9.0780735E-01 3.6856958E+00 4.5348266E+00 8.3303180E+00 7.4253452E+00 1.4002219E+01 1.1858903E+01
# time = 4.5000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 9 10
0.000000E+00 7.9301425E+00 2.3544877E+00
0.000000E+00 7.9301425E+00 2.3544877E+00
0.000000E+00 7.9301425E+00 2.3544877E+00
# time = 4.6000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 1 2 3 4 5 6 7 8
0.000000E+00 2.3643429E+00 5.4002524E+00 9.095070E-01 3.7055095E+00 4.5523608E+00 8.4511173E+00 7.4880148E+00 1.4305476E+01 1.2044388E+01
0.000000E+00 2.3643429E+00 5.4002524E+00 9.095070E-01 3.7055095E+00 4.5523608E+00 8.4511173E+00 7.4880148E+00 1.4305476E+01 1.2044388E+01
0.000000E+00 2.3643429E+00 5.4002524E+00 9.095070E-01 3.7055095E+00 4.5523608E+00 8.4511173E+00 7.4880148E+00 1.4305476E+01 1.2044388E+01
# time = 4.6000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 9 10
0.000000E+00 8.0491252E+00 2.3643429E+00
0.000000E+00 8.0491252E+00 2.3643429E+00
0.000000E+00 8.0491252E+00 2.3643429E+00
# time = 4.7000E-14 : depth vs zbar
s r zbar zbar zbar zbar zbar zbar zbar zbar
s 1 2 3 4 5 6 7 8
0.000000E+00 2.3738416E+00 5.4241912E+00 9.1201545E-01 3.7254945E+00 4.5693760E+00 8.5694939E+00 7.5490548E+00 1.4610726E+01 1.2255765E+01
```

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0.000000E+00 2.3738416E+00 5.4241912E+00 9.1201545E-01 3.7254945E+00 4.5693760E+00 8.5694893E+00 7.5490548E+00 1.4610726E+01 1.2225576E+01
0.000000E+00 2.3738416E+00 5.4241912E+00 9.1201545E-01 3.7254945E+00 4.5693760E+00 8.5694893E+00 7.5490548E+00 1.4610726E+01 1.2225576E+01
# time = 4.7000E-14 : depth vs zbar
$ r zbar zbar
$ 9 10
0.000000E+00 8.1638681E+00 2.3738416E+00
0.000000E+00 8.1638681E+00 2.3738416E+00
0.000000E+00 8.1638681E+00 2.3738416E+00
# time = 4.8000E-14 : depth vs zbar
$ r zbar zbar zbar zbar zbar zbar zbar zbar
$ 9 10 1 2 3 4 5 6 7 8
0.000000E+00 2.3830444E+00 5.4471741E+00 9.1400132E-01 3.7456670E+00 4.5858942E+00 8.6855509E+00 7.6885932E+00 1.4911717E+01 1.2403366E+01
0.000000E+00 2.3830444E+00 5.4471741E+00 9.1400132E-01 3.7456670E+00 4.5858942E+00 8.6855509E+00 7.6885932E+00 1.4911717E+01 1.2403366E+01
0.000000E+00 2.3830444E+00 5.4471741E+00 9.1400132E-01 3.7456670E+00 4.5858942E+00 8.6855509E+00 7.6885932E+00 1.4911717E+01 1.2403366E+01
# time = 4.8000E-14 : depth vs zbar
$ r zbar zbar zbar zbar zbar zbar zbar zbar
$ 9 10 1 2 3 4 5 6 7 8
0.000000E+00 8.2762214E+00 2.3830444E+00
0.000000E+00 8.2762214E+00 2.3830444E+00
0.000000E+00 8.2762214E+00 2.3830444E+00
# time = 4.9000E-14 : depth vs zbar
$ r zbar zbar zbar zbar zbar zbar zbar zbar
$ 9 10 1 2 3 4 5 6 7 8
0.000000E+00 2.3919678E+00 5.4692454E+00 9.1591120E-01 3.7660529E+00 4.6019536E+00 8.8004063E+00 7.6667435E+00 1.5223993E+01 1.2576380E+01
0.000000E+00 2.3919678E+00 5.4692454E+00 9.1591120E-01 3.7660529E+00 4.6019536E+00 8.8004063E+00 7.6667435E+00 1.5223993E+01 1.2576380E+01
0.000000E+00 2.3919678E+00 5.4692454E+00 9.1591120E-01 3.7660529E+00 4.6019536E+00 8.8004063E+00 7.6667435E+00 1.5223993E+01 1.2576380E+01
# time = 4.9000E-14 : depth vs zbar
$ r zbar zbar zbar zbar zbar zbar zbar zbar
$ 9 10 1 2 3 4 5 6 7 8
0.000000E+00 8.3837099E+00 2.3919678E+00
0.000000E+00 8.3837099E+00 2.3919678E+00
0.000000E+00 8.3837099E+00 2.3919678E+00
# time = 5.0000E-14 : depth vs zbar
$ r zbar zbar zbar zbar zbar zbar zbar zbar
$ 9 10 1 2 3 4 5 6 7 8
0.000000E+00 2.4006270E+00 5.4904510E+00 9.1774795E-01 3.7866730E+00 4.6175910E+00 8.9121374E+00 7.7236092E+00 1.5530354E+01 1.2745722E+01
0.000000E+00 2.4006270E+00 5.4904510E+00 9.1774795E-01 3.7866730E+00 4.6175910E+00 8.9121374E+00 7.7236092E+00 1.5530354E+01 1.2745722E+01
0.000000E+00 2.4006270E+00 5.4904510E+00 9.1774795E-01 3.7866730E+00 4.6175910E+00 8.9121374E+00 7.7236092E+00 1.5530354E+01 1.2745722E+01
# time = 5.0000E-14 : depth vs zbar
$ r zbar zbar zbar zbar zbar zbar zbar zbar
$ 9 10 1 2 3 4 5 6 7 8
0.000000E+00 8.4881038E+00 2.4006270E+00
0.000000E+00 8.4881038E+00 2.4006270E+00
0.000000E+00 8.4881038E+00 2.4006270E+00

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2 Input / output for TDAP/Siesta calculations associated with figure 7

A full account of input and output data for TDAP/Siesta calculations associated with figure 7 can be found on Zenodo using DOI: [10.5281/zenodo.3909424](https://doi.org/10.5281/zenodo.3909424)